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(*E*)-1-(1,3-Benzodioxol-5-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one

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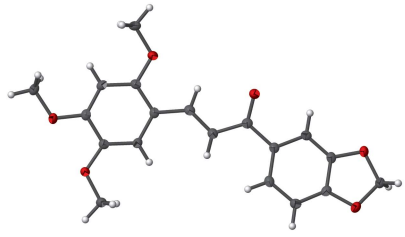
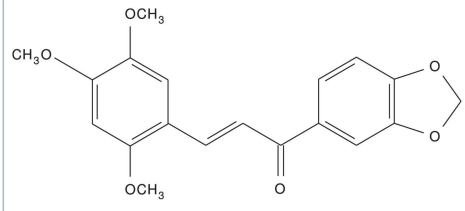
The molecule of the title compound $C_{19}H_{18}O_6$, adopts an *E* conformation about the C=C double bond and the C—C=C—C torsion angle is −179.30 (16)°. The molecule is nearly planar, as indicated by the dihedral angle of 6.99 (6)° between the benzene ring and the benzodioxalane ring. In the crystal, molecules are linked *via* weak C—H···O hydrogen bonds, forming zigzag chains propagating along the *b* axis.

3D view



Chemical scheme



Structure description

Chalcones form the central core for the construction of a variety of bioactive compounds. The usual method for the synthesis of chalcones involves the condensation of an aromatic aldehyde and an aromatic ketone in the presence of aqueous alkaline bases (Naveen *et al.*, 2016). Chalcones and their derivatives demonstrate a wide range of biological activities such as anti-diabetic, antineoplastic, antihypertensive, anti-inflammatory, anti-malarial, antioxidant and antifungal activities (Mahapatra *et al.*, 2015). The α,β-unsaturated carbonyl system of chalcones made them useful building blocks in organic synthesis. They have been efficiently employed as precursors in the syntheses of biologically potent benzothiazepines (Manjunath *et al.*, 2014). In view of diversified applications of chalcones and as a part of our ongoing work on such molecules (Tejkiran *et al.*, 2016), we report herein the synthesis and crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. The molecule is nearly planar with a dihedral angle of 6.99 (6)° between the benzene and benzodioxalane

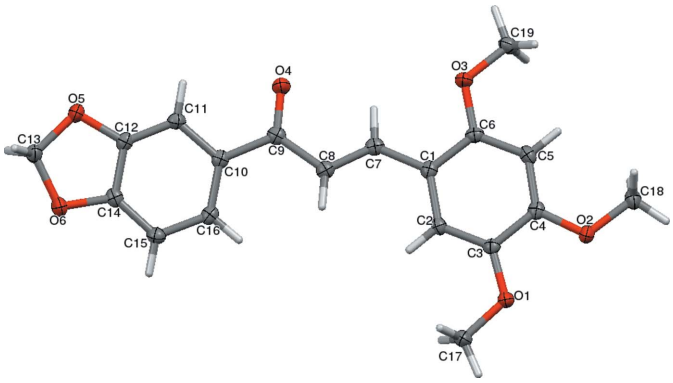


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

rings that are bridged by the olefinic double bond. This value is less than the value of 19.13 (15)° between the aromatic rings in the related chalcone derivative (*E*)-3-(2,3-dichlorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (Naveen *et al.*, 2016). The *trans* conformation of the C7═C8 double bond in the central enone group is confirmed by the value of the C1—C7═C8—C9 torsion angle −179.30 (16)°. The methoxy groups at C3, C4 and C6 are nearly coplanar with the C1–C6 benzene ring. In the crystal, the molecules are linked *via* weak C—H···O hydrogen bonds (Table 1), forming zigzag chains parallel to the *b* axis (Fig. 2).

Synthesis and crystallization

A mixture of 2,4,5-trimethoxybenzaldehyde (5 mmol), 1-(benzo[*d*][1,3]dioxol-5-yl)ethanone (5 mmol) and sodium hydroxide (5 mmol) in 95% ethyl alcohol (25 ml) was stirred at room temperature for 3 h. The progress of the reaction was monitored by TLC. After completion of the reaction, the mixture was poured into ice cold water and kept in the refrigerator overnight. The solid that formed was filtered, and washed with cold hydrochloric acid (5%). Yellow rectangular crystals were obtained by slow evaporation of a solution in methanol (yield 89%, m.p. 399–401 K).

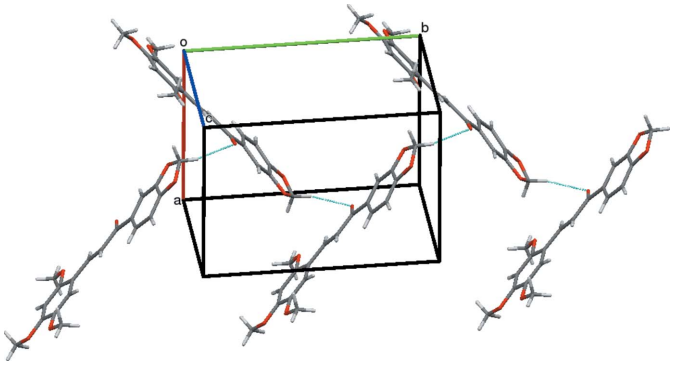


Figure 2
Partial packing diagram of the title compound, showing the formation of a molecular chain parallel to the *b* axis *via* C—H···O hydrogen bonds (dotted lines).

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*B*···O4^{i}	0.97	2.54	3.464 (2)	159

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{18}O_6$
M_r	342.33
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, *b*, *c* (Å)	10.9127 (2), 13.4406 (3), 11.1011 (2)
β (°)	106.287 (1)
V (Å^3)	1562.89 (5)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.91
Crystal size (mm)	0.29 × 0.26 × 0.24
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2011)
T_{min}, T_{max}	0.779, 0.812
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12593, 2568, 2283
R_{int}	0.054
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.586
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.145, 1.09
No. of reflections	2568
No. of parameters	229
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.30

Computer programs: *APEX2* and *SAINT* (Bruker, 2011), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x162026 [https://doi.org/10.1107/S2414314616020265]

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Crystal data

$C_{19}H_{18}O_6$
M_r = 342.33
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.9127 (2) Å
b = 13.4406 (3) Å
c = 11.1011 (2) Å
β = 106.287 (1)°
V = 1562.89 (5) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.455 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2568 reflections
θ = 5.3–64.5°
μ = 0.91 mm^{-1}
T = 296 K
Block, yellow
0.29 × 0.26 × 0.24 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2011)
T_{min} = 0.779, T_{max} = 0.812
12593 measured reflections
2568 independent reflections
2283 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 64.5°, θ_{min} = 5.3°
h = −11→12
k = −15→15
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.145
S = 1.09
2568 reflections
229 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1062P)^2 + 0.0554P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.91113 (10)	1.12891 (8)	1.26097 (10)	0.0195 (3)
O2	1.03766 (10)	1.20902 (8)	1.12453 (10)	0.0211 (3)
O3	0.78978 (11)	1.03030 (9)	0.75876 (10)	0.0253 (4)
O4	0.48629 (11)	0.80424 (9)	0.74724 (10)	0.0256 (4)
O5	0.11332 (10)	0.58892 (9)	0.77554 (10)	0.0225 (3)
O6	0.11852 (11)	0.57683 (9)	0.98559 (11)	0.0239 (4)
C1	0.75134 (14)	1.00721 (11)	0.95591 (15)	0.0168 (5)
C2	0.77990 (14)	1.03224 (11)	1.08453 (14)	0.0166 (5)
C3	0.87534 (14)	1.09951 (12)	1.13825 (14)	0.0170 (5)
C4	0.94560 (14)	1.14401 (11)	1.06326 (15)	0.0173 (5)
C5	0.91856 (15)	1.12160 (11)	0.93735 (15)	0.0186 (5)
C6	0.82250 (15)	1.05351 (12)	0.88408 (14)	0.0179 (5)
C7	0.65492 (15)	0.93450 (11)	0.89609 (15)	0.0179 (5)
C8	0.57013 (15)	0.88508 (11)	0.94087 (15)	0.0184 (5)
C9	0.48403 (14)	0.81406 (12)	0.85739 (15)	0.0185 (5)
C10	0.39080 (14)	0.75351 (11)	0.90211 (14)	0.0167 (4)
C11	0.29852 (14)	0.70065 (11)	0.80904 (14)	0.0180 (5)
C12	0.21113 (14)	0.64612 (11)	0.84800 (15)	0.0174 (5)
C13	0.04917 (16)	0.54733 (12)	0.86066 (15)	0.0218 (5)
C14	0.21371 (15)	0.63905 (11)	0.97324 (15)	0.0178 (5)
C15	0.30402 (15)	0.68775 (12)	1.06610 (15)	0.0198 (5)
C16	0.39221 (15)	0.74662 (12)	1.02786 (15)	0.0183 (5)
C17	0.84472 (16)	1.08758 (13)	1.34227 (15)	0.0234 (5)
C18	1.11336 (15)	1.25347 (13)	1.05277 (15)	0.0227 (5)
C19	0.87351 (16)	1.06180 (12)	0.68832 (15)	0.0226 (5)
H2	0.73360	1.00290	1.13380	0.0200*
H5	0.96430	1.15180	0.88820	0.0220*
H7	0.65140	0.91980	0.81330	0.0220*
H8	0.56590	0.89550	1.02240	0.0220*
H11	0.29740	0.70290	0.72500	0.0210*
H13A	−0.03790	0.57170	0.84070	0.0260*
H13B	0.04680	0.47540	0.85400	0.0260*
H15	0.30640	0.68190	1.15020	0.0240*
H16	0.45330	0.78200	1.08790	0.0220*
H17A	0.75530	1.10180	1.31010	0.0350*
H17B	0.87660	1.11610	1.42440	0.0350*
H17C	0.85740	1.01680	1.34720	0.0350*
H18A	1.15250	1.20220	1.01600	0.0340*
H18B	1.17840	1.29410	1.10660	0.0340*

H18C	1.06000	1.29390	0.98760	0.0340*
H19A	0.87440	1.13320	0.68500	0.0340*
H19B	0.84450	1.03560	0.60470	0.0340*
H19C	0.95820	1.03790	0.72780	0.0340*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0220 (6)	0.0216 (6)	0.0148 (6)	−0.0055 (4)	0.0049 (5)	−0.0011 (4)
O2	0.0203 (6)	0.0225 (6)	0.0193 (6)	−0.0070 (4)	0.0035 (5)	−0.0002 (4)
O3	0.0311 (7)	0.0300 (7)	0.0164 (6)	−0.0111 (5)	0.0094 (5)	−0.0039 (5)
O4	0.0303 (7)	0.0282 (7)	0.0202 (6)	−0.0094 (5)	0.0104 (5)	−0.0053 (5)
O5	0.0215 (6)	0.0247 (6)	0.0206 (6)	−0.0080 (5)	0.0047 (5)	−0.0030 (5)
O6	0.0209 (6)	0.0287 (7)	0.0230 (7)	−0.0076 (5)	0.0077 (5)	0.0005 (5)
C1	0.0151 (8)	0.0146 (8)	0.0198 (8)	0.0023 (6)	0.0033 (6)	0.0010 (6)
C2	0.0159 (8)	0.0152 (8)	0.0194 (8)	0.0004 (6)	0.0061 (6)	0.0013 (6)
C3	0.0166 (8)	0.0177 (8)	0.0162 (8)	0.0020 (6)	0.0037 (6)	0.0009 (6)
C4	0.0151 (8)	0.0145 (8)	0.0211 (9)	0.0020 (6)	0.0032 (6)	0.0016 (6)
C5	0.0178 (8)	0.0178 (8)	0.0216 (9)	0.0014 (6)	0.0080 (6)	0.0038 (6)
C6	0.0189 (8)	0.0187 (8)	0.0158 (8)	0.0024 (6)	0.0044 (7)	−0.0006 (6)
C7	0.0183 (8)	0.0166 (8)	0.0184 (8)	0.0045 (6)	0.0043 (6)	0.0003 (6)
C8	0.0187 (8)	0.0171 (8)	0.0190 (8)	0.0019 (6)	0.0046 (7)	−0.0004 (6)
C9	0.0190 (8)	0.0164 (8)	0.0205 (9)	0.0043 (6)	0.0063 (7)	0.0011 (6)
C10	0.0165 (8)	0.0131 (7)	0.0202 (8)	0.0033 (6)	0.0046 (6)	0.0002 (6)
C11	0.0206 (8)	0.0167 (8)	0.0167 (8)	0.0022 (6)	0.0054 (7)	0.0000 (6)
C12	0.0159 (7)	0.0141 (8)	0.0214 (9)	0.0016 (6)	0.0039 (6)	−0.0020 (6)
C13	0.0205 (8)	0.0237 (9)	0.0226 (9)	−0.0055 (7)	0.0082 (7)	−0.0034 (7)
C14	0.0164 (8)	0.0153 (8)	0.0228 (9)	0.0031 (6)	0.0073 (6)	0.0018 (6)
C15	0.0205 (8)	0.0212 (9)	0.0178 (8)	0.0021 (6)	0.0054 (7)	0.0013 (6)
C16	0.0168 (8)	0.0158 (8)	0.0206 (9)	0.0025 (6)	0.0025 (6)	−0.0009 (6)
C17	0.0271 (9)	0.0264 (9)	0.0177 (9)	−0.0070 (7)	0.0079 (7)	−0.0006 (6)
C18	0.0196 (9)	0.0225 (9)	0.0266 (9)	−0.0038 (7)	0.0076 (7)	0.0011 (7)
C19	0.0281 (9)	0.0234 (9)	0.0187 (9)	−0.0001 (7)	0.0107 (7)	0.0005 (6)

Geometric parameters (Å, º)

O1—C3	1.3661 (18)	C11—C12	1.366 (2)
O1—C17	1.420 (2)	C12—C14	1.386 (2)
O2—C4	1.3609 (19)	C14—C15	1.376 (2)
O2—C18	1.429 (2)	C15—C16	1.401 (2)
O3—C6	1.3717 (18)	C2—H2	0.9300
O3—C19	1.424 (2)	C5—H5	0.9300
O4—C9	1.2370 (19)	C7—H7	0.9300
O5—C12	1.3769 (19)	C8—H8	0.9300
O5—C13	1.438 (2)	C11—H11	0.9300
O6—C13	1.437 (2)	C13—H13A	0.9700
O6—C14	1.370 (2)	C13—H13B	0.9700
C1—C2	1.414 (2)	C15—H15	0.9300

C1—C6	1.405 (2)	C16—H16	0.9300
C1—C7	1.453 (2)	C17—H17A	0.9600
C2—C3	1.382 (2)	C17—H17B	0.9600
C3—C4	1.413 (2)	C17—H17C	0.9600
C4—C5	1.379 (2)	C18—H18A	0.9600
C5—C6	1.392 (2)	C18—H18B	0.9600
C7—C8	1.343 (2)	C18—H18C	0.9600
C8—C9	1.471 (2)	C19—H19A	0.9600
C9—C10	1.492 (2)	C19—H19B	0.9600
C10—C11	1.415 (2)	C19—H19C	0.9600
C10—C16	1.395 (2)		

C3—O1—C17	117.82 (12)	C1—C2—H2	119.00
C4—O2—C18	116.80 (12)	C3—C2—H2	119.00
C6—O3—C19	117.70 (13)	C4—C5—H5	120.00
C12—O5—C13	105.89 (12)	C6—C5—H5	120.00
C13—O6—C14	106.30 (12)	C1—C7—H7	115.00
C2—C1—C6	117.87 (14)	C8—C7—H7	115.00
C2—C1—C7	123.22 (14)	C7—C8—H8	121.00
C6—C1—C7	118.90 (14)	C9—C8—H8	121.00
C1—C2—C3	121.16 (14)	C10—C11—H11	121.00
O1—C3—C2	126.14 (14)	C12—C11—H11	121.00
O1—C3—C4	114.49 (14)	O5—C13—H13A	110.00
C2—C3—C4	119.38 (14)	O5—C13—H13B	110.00
O2—C4—C3	115.07 (14)	O6—C13—H13A	110.00
O2—C4—C5	124.41 (14)	O6—C13—H13B	110.00
C3—C4—C5	120.51 (14)	H13A—C13—H13B	108.00
C4—C5—C6	119.73 (15)	C14—C15—H15	122.00
O3—C6—C1	116.54 (14)	C16—C15—H15	122.00
O3—C6—C5	122.08 (14)	C10—C16—H16	119.00
C1—C6—C5	121.35 (14)	C15—C16—H16	119.00
C1—C7—C8	130.50 (15)	O1—C17—H17A	109.00
C7—C8—C9	118.20 (14)	O1—C17—H17B	110.00
O4—C9—C8	120.37 (15)	O1—C17—H17C	109.00
O4—C9—C10	118.37 (14)	H17A—C17—H17B	110.00
C8—C9—C10	121.25 (14)	H17A—C17—H17C	109.00
C9—C10—C11	116.28 (13)	H17B—C17—H17C	109.00
C9—C10—C16	123.50 (14)	O2—C18—H18A	109.00
C11—C10—C16	120.21 (14)	O2—C18—H18B	109.00
C10—C11—C12	117.09 (14)	O2—C18—H18C	109.00
O5—C12—C11	127.62 (14)	H18A—C18—H18B	109.00
O5—C12—C14	110.01 (13)	H18A—C18—H18C	110.00
C11—C12—C14	122.34 (15)	H18B—C18—H18C	109.00
O5—C13—O6	107.78 (13)	O3—C19—H19A	109.00
O6—C14—C12	109.85 (14)	O3—C19—H19B	109.00
O6—C14—C15	128.27 (15)	O3—C19—H19C	109.00
C12—C14—C15	121.86 (15)	H19A—C19—H19B	109.00
C14—C15—C16	116.77 (15)	H19A—C19—H19C	109.00

C10—C16—C15	121.68 (15)	H19B—C19—H19C	109.00
C17—O1—C3—C2	−0.3 (2)	C2—C3—C4—C5	0.7 (2)
C17—O1—C3—C4	179.87 (13)	O2—C4—C5—C6	179.72 (14)
C18—O2—C4—C3	178.25 (13)	C3—C4—C5—C6	−0.9 (2)
C18—O2—C4—C5	−2.4 (2)	C4—C5—C6—O3	178.47 (15)
C19—O3—C6—C1	−169.19 (14)	C4—C5—C6—C1	0.4 (2)
C19—O3—C6—C5	12.7 (2)	C1—C7—C8—C9	−179.30 (16)
C13—O5—C12—C11	−179.87 (15)	C7—C8—C9—O4	−3.4 (2)
C13—O5—C12—C14	2.25 (17)	C7—C8—C9—C10	177.58 (15)
C12—O5—C13—O6	−3.93 (16)	O4—C9—C10—C11	−9.5 (2)
C14—O6—C13—O5	4.16 (16)	O4—C9—C10—C16	169.88 (15)
C13—O6—C14—C12	−2.82 (17)	C8—C9—C10—C11	169.58 (14)
C13—O6—C14—C15	178.86 (16)	C8—C9—C10—C16	−11.1 (2)
C6—C1—C2—C3	−0.5 (2)	C9—C10—C11—C12	−178.97 (14)
C7—C1—C2—C3	177.87 (15)	C16—C10—C11—C12	1.7 (2)
C2—C1—C6—O3	−177.88 (14)	C9—C10—C16—C15	−179.06 (15)
C2—C1—C6—C5	0.3 (2)	C11—C10—C16—C15	0.2 (2)
C7—C1—C6—O3	3.7 (2)	C10—C11—C12—O5	−179.86 (14)
C7—C1—C6—C5	−178.14 (15)	C10—C11—C12—C14	−2.2 (2)
C2—C1—C7—C8	6.3 (3)	O5—C12—C14—O6	0.37 (18)
C6—C1—C7—C8	−175.42 (17)	O5—C12—C14—C15	178.81 (14)
C1—C2—C3—O1	−179.85 (14)	C11—C12—C14—O6	−177.65 (14)
C1—C2—C3—C4	0.0 (2)	C11—C12—C14—C15	0.8 (2)
O1—C3—C4—O2	0.0 (2)	O6—C14—C15—C16	179.32 (15)
O1—C3—C4—C5	−179.42 (14)	C12—C14—C15—C16	1.2 (2)
C2—C3—C4—O2	−179.86 (14)	C14—C15—C16—C10	−1.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*B*···O4^{i}	0.97	2.54	3.464 (2)	159

Symmetry code: (i) −*x*+1/2, *y*−1/2, −*z*+3/2.